*Journal of Statistical Physics, Vol. 35, Nos. 5/6, 1984*

# A Geometric Interpretation of the Roughening Transition in Ising Models

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*Received June 20, 1983, revision received January 10, 1984*

Progress in the area of the Ising model roughening transition has previously been limited by the lack of a good definition for the interface separating the pure phases. In the present work, a graphical definition is introduced and it is shown that roughening occurs precisely when this interface fluctuates to infinity.

**KEY WORDS:** Roughening transition; Ising model.

## 1. INTRODUCTION

In 1972, Dobrushin[1] showed that at low temperature in dimensions greater than 2, the two phases of an Ising model can coexist in an equilibrium state which is not translation invariant. Three years later this result was extended and greatly simplified by van Beijeren,[2] who used correlation inequalities to show that in $d$ dimensions the phase coexistence is stable at least up to the $(d-1)$-dimensional critical temperature.

Since the one-dimensional critical temperature is zero, that argument gives no information about two dimensions, and indeed it has been shown[3,4] that all the Gibbs states of the two-dimensional Ising model are convex combinations of the two pure phases (and, thus, translation invariant).

In the theory of crystal growth, it was postulated, by Burton and Cabrera[5] (1949) that the surface structure of a crystal, which is in equilibrium with its vapour, would be radically different depending on

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0022-4715/84/0600-0473$03.50/0 

whether it was grown above or below a "roughening" temperature. In the context of the Ising model the corresponding question is whether in dimension greater than 2, the existence of states which are not translation invariant persists up to the critical temperature of the model, $T_c$, or whether there exists an intermediate roughening temperature, $T_R$, above which all states are translation invariant.

Let $\Lambda_{L,M}$ be the box of height $2M+1$ and cross section $(2L+1)^{d-1}$ centered at the origin in $Z^d$.

$$\Lambda_{L,M} = \{ i \in Z^d \mid -M \leqslant i_1 \leqslant M,\ -L \leqslant i_\alpha \leqslant L, \alpha = 2, \ldots, d \}$$

A natural way to impose phase coexistence is by the $\pm$ boundary conditions, which were studied by Dobrushin. These amount to setting all of the spins in $\Lambda_{L,M}^c$ with $i_1 \geqslant 0$ to be $+1$, and those for which $i_1 < 0$ to be $-1$. In the case of a nearest-neighbor interaction, which will be considered here, it is only necessary to fix those spins in $\Lambda_{L,M}^c$ which have a nearest-neighbor in $\Lambda_{L,M}$.

Let $\langle \cdot \rangle_{L,M}^{\pm}$ denote the Gibbs state induced in $\Lambda_{L,M}$ by the $\pm$ boundary conditions, and denote by $\langle \cdot \rangle^{\pm}$, the state obtained by taking

$$\lim_{L\to\infty} \lim_{M\to\infty} \langle \cdot \rangle_{L,M}^{\pm}$$

The roughening temperature $T_R$ is defined as

$$\sup\{ T \mid \text{at the temperature } T \text{ the state } \langle \cdot \rangle^{\pm} \text{ is not translation invariant} \}$$

Clearly $T_R \leqslant T_c$. The main open question is whether there is a strict inequality in dimensions greater than 2. The expectation is that $T_{R,3} < T_{c,3}$ yet $T_{R,d} = T_{c,d}$ for $d \geqslant 4$.

The $\langle \cdot \rangle^{\pm}$ state is translation invariant if and only if the spontaneous magnetization vanishes. This was first shown by Messager and Miracle-Sole,[6] who used correlation inequalities. However it is also a simple consequence of the Holley version[7] of the FKG inequality[8] and the observation that the "shift" of the $\langle \cdot \rangle^{\pm}$ state in the positive $i_1$ direction makes the state more positive in the FKG sense.

The expected mechanism for roughening is the following: at low temperatures one has a stable interface separating the pure phases. As the temperature is raised, the interface fluctuations increase and become unbounded at the roughening temperature $T_R$. For $T_R < T < T_c$, the interface would be found either far above or far below the origin, and the resulting state would be $(\mu_+ + \mu_-)/2$.

Progress in this area has been limited by the lack of a good definition for the interface separating the pure phase. In this paper a graphical definition is introduced and it is shown that roughening corresponds precisely to the fluctuation of this interface to infinity.

Before proceeding, let us briefly describe the inadequacy of the existing method for describing the interface.

Consider the state $\langle \cdot \rangle^{\pm}_{L,M}$. If one associates spin configurations with contours in the usual way, then the $\pm$ boundary conditions impose the existence of one long contour (or surface in dimension greater than 2) which is "tied down" at the $i_1 = -1/2$ plane. This long contour is usually taken as the interface between the pure phases.

This procedure was used by Dobrushin in his seminal work, and also in the proof of translation invariance in two dimensions. However, any candidate for the interface of phase separation should have the property that in the pure phases such surfaces do not occur. In two dimensions, the contours mentioned above do have this property, as was shown by Russo.[9] It is expected, however, that in the three-dimensional "plus" state infinite negative clusters will appear at temperatures above a "percolation" temperature $T_{p,3}$ which is below $T_{c,3}$. If so, then above $T_{p,3}$ even the pure phases of the three-dimensional system would contain infinite contours. We therefore consider that these contours provide an unsatisfactory description of the interface of phase separation in three and more dimensions.

It is conjectured that $T_{R,3} < T_{p,3}$. Bricmont, Fontaine, and Lebowitz[10] have analyzed the consequences of this conjecture, and developed a description of roughening based on it.

In Section 2 we introduce a model of the interface in the Ising system. Our main result, which is in Section 3, is a theorem establishing the correspondence between the destabilization of this surface and the roughening transition.

Thus, while the main issue is still unresolved, we show how it can be given an exact geometrical formulation.

## 2. DESCRIPTION OF THE INTERFACE

Throughout this paper, we are considering the nearest-neighbor Ising system. We begin this section with a brief review of a graphical method. The reader is referred to Refs. 11 and 12 and references cited therein for a more complete introduction.

The system consists of spin variables, $\sigma_i = \pm 1$, associated with lattice sites $i \in Z^d$. Let $\Lambda \subseteq Z^d$ be a finite box. In the case of "free" boundary conditions, the Hamiltonian in $\Lambda$ is given by

$$-H_{\Lambda,\mathrm{free}} = \sum_{\substack{\langle ij \rangle \\ i,j \in \Lambda}} J\sigma_i\sigma_j$$

where $J > 0$, and the symbol $\langle ij \rangle$ indicates a sum over nearest-neighbor pairs.

Each pair of nearest-neighbor sites will be referred to as a bond. The collection of all bonds will be denoted by $B$.

The partition function $Z$ is given by

$$Z = \sum_{\sigma_i = \pm 1} \prod_{\langle ij \rangle} e^{BJ\sigma_i\sigma_j}$$

By expanding the exponentials

$$e^{BJ\sigma_i\sigma_j} = \sum_{n_b=0}^{\infty} (\beta J)^{n_b} (\sigma_i\sigma_j)^{n_b} / n_b!$$

and averaging over the $\{\sigma_i\}$, one obtains

$$Z = \sum_{\partial \mathbf{n} = \phi} W(\mathbf{n})$$

where $\mathbf{n}$ is an assignment of nonnegative integers to the bonds, and the weight $W(\mathbf{n})$ is given by

$$W(\mathbf{n}) = \prod_{b \in B} (\beta J)^{n_b} / n_b!$$

It is convenient to view $\{n_b\}$ as the unoriented fluxes of a current, and we regard

$$\partial \mathbf{n} = \left\{ i \in \Lambda \,|\, (-1)^{\sum_{b \ni i} n_b} = -1 \right\}$$

as the set of sources of the flux configuration $\mathbf{n}$.

For the correlation function $\langle \sigma_K \rangle$, with $\sigma_K = \prod_{k \in K} \sigma_k$, a similar expansion leads to

$$\langle \sigma_K \rangle = \sum_{\partial \mathbf{n} = K} W(\mathbf{n}) \Big/ \sum_{\partial \mathbf{n} = \phi} W(\mathbf{n})$$

An assignment of fluxes $\mathbf{n}$ will sometimes be called a graph. We will say that $\mathbf{s}$ is a subgraph of $\mathbf{n}$ ($\mathbf{s} \leqslant \mathbf{n}$) if and only if $s_b \leqslant n_b$ for all $b$.

A path from $j$ to $k$ is a collection of bonds $b_1, \ldots, b_s$ such that $b_1 \ni j$, $b_s \ni k$ and $b_i$ and $b_{i+1}$ have a site in common for $i = 1, \ldots, s-1$.

We will say that $\mathbf{n}$ contains a path from $j$ to $k$ if there exists a path $b_1, \ldots, b_s$ from $j$ to $k$ for which $n_{b_i} > 0$ for $i = 1, \ldots, s$.

An important tool is provided by the following result of Griffiths, Hurst, and Sherman.[13]

**Lemma** (GHS). Let $K_1$ and $K_2$ be sets of sites. Then

$$\sum_{\substack{\partial \mathbf{n}_1 = K_1 \\ \partial \mathbf{n}_2 = K_2}} W(\mathbf{n}_1) W(\mathbf{n}_2) = \sum_{\substack{\partial \mathbf{n}_1 = K_1 \Delta K_2 \\ \partial \mathbf{n}_2 = \phi}}{}' \; W(\mathbf{n}_1) W(\mathbf{n}_2)$$

where the primed summation has the restriction that $\mathbf{n}_1 + \mathbf{n}_2$ contains a subgraph $\mathbf{s}$ with $\partial \mathbf{s} = K_2$. ($\Delta$ indicates the usual symmetric difference.)

We next consider the case of plus boundary conditions. The Hamiltonian in $\Lambda$ is now

$$-H_{\Lambda,+} = \sum_{\substack{\langle ij\rangle \\ i,j\in\Lambda}} J\sigma_i\sigma_j + \sum_{\substack{\langle ij\rangle \\ i\in\Lambda, j\in\Lambda^c}} J\sigma_i$$

and the partition function is given by

$$Z_{\Lambda,+} = \sum_{\sigma_i=\pm 1} \prod_{\substack{\langle ij\rangle \\ i,j\in\Lambda}} e^{\beta J\sigma_i\sigma_j} \prod_{\substack{\langle ij\rangle \\ i\in\Lambda, j\in\Lambda^c}} e^{\beta J\sigma_i}$$

There are now two types of bonds: those contained entirely in $\Lambda$, and those linking $\Lambda$ with $\Lambda^c$.

Define

$$\partial\Lambda = \{ j \in \Lambda^c \mid \text{there exists } i \in \Lambda \text{ with } |i-j| = 1 \}$$

Expanding the exponentials as before one obtains

$$Z_{\Lambda,+} = \sum_{\partial\mathbf{n}\setminus\partial\Lambda=\phi} W(\mathbf{n})$$

Note that now $\mathbf{n}$ is allowed to have sources, but only in $\partial\Lambda$.

One obtains a similar expression for the correlation functions.

Finally, let us consider general boundary conditions, which are obtained by specifying a mixed configuration of spins in $\partial\Lambda$.

Parametrizing the boundary spin configuration by $\gamma$, one obtains

$$Z_{\Lambda,\gamma} = \sum_{\partial\mathbf{n}\setminus\partial\Lambda=\phi} W(\mathbf{n})(-1)^{n_-(\gamma)}$$

where $n_-(\gamma)$ is the sum of fluxes going into negative boundary spins.

Let us now turn to a discussion of the interface.

As in Section 1, we consider

$$\Lambda_{L,M} = \{ i \in Z^d \mid -M \leqslant i_1 \leqslant M,\ -L \leqslant i_\alpha \leqslant L,\ \alpha = 2, \ldots, d \}$$

and the $\pm$boundary conditions defined by fixing all of the spins in $\partial\Lambda_{L,M}$ for which $i_1 \geqslant 0$ to be $+1$, and those for which $i_1 < 0$ to be $-1$.

One has the following expression for the partition function in $\Lambda_{L,M}$ with $\pm$ boundary conditions:

$$Z^{\pm}_{L,M} = \sum_{\partial\mathbf{n}\setminus\partial\Lambda=\phi} W(\mathbf{n})(-1)^{n_-}$$

where $n_-$ is the sum of fluxes going into boundary sites with $i_1 < 0$.

Graphical methods will now be used to write this expression in a manifestly positive form.

We will denote the collection of bonds which contain at least one site with $i_1 < 0$ by $B'$. The flux configuration in this region will be denoted by $\mathbf{n}'$. The remainder of the flux configuration will be denoted by $\mathbf{n}$ as before.

Using these conventions, we can write

$$Z^{\pm}_{L,M} = \sum_{\partial(\mathbf{n}+\mathbf{n}')\setminus\partial\Lambda=\phi} W(\mathbf{n})W(\mathbf{n}')(-1)^{n'_-} \tag{2.1}$$

where $n'_-$ is defined in the same way as $n_-$.

We superimpose the bottom half of $\Lambda_{L,M}$ on the top half by reflecting $(i_1, i_2, \ldots, i_d) \to (-i_1, i_2, \ldots, i_d)$ for sites with $i_1 < 0$. This procedure is illustrated in two dimensions in Fig. 1.

In this manner, bonds in the lower half of $\Lambda_{L,M}$ are paired with bonds in the upper half. Only bonds in the hyperplane $i_1 = 0$ are unpaired. We will call this hyperplane $P_0$.

We evaluate (2.1) by first summing over $\mathbf{m} \equiv \mathbf{n} + \mathbf{n}'$, where we now view $\mathbf{n}'$ as the reflected source configuration and not the original one in the bottom half of the box. Note that $\mathbf{n}$ and $\mathbf{n}'$ are allowed to have sources at the hyperplane $P_0$: the condition is only that $\mathbf{m}$ have no sources there.

The expression (2.1) may be written

$$\sum_{\partial\mathbf{m}\setminus\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\setminus(\partial\Lambda\, U P_0)=\phi}} \prod_{b\in B'} \binom{m_b}{n'_b}(-1)^{n'_-} \tag{2.2}$$

Suppose that $\mathbf{m}$ contains a path connecting a boundary site with $i_1 \neq 0$ to $P_0$. Then we claim that the sum over $\mathbf{n}'$ in (2.2) is zero. To show this, we will use the symmetric difference trick as in Ref. 11.

With the given $\mathbf{m}$, we associate a graph $\mathbf{M}$ which, for each $b = \{x, y\}$, consists of $m_b$ distinct lines connecting the sites $x$ and $y$. We will use the

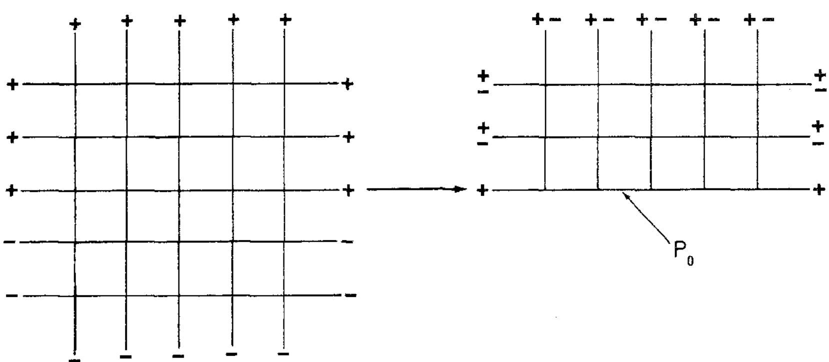


Fig. 1. Superposition of the bottom half of $\Lambda_{L,M}$ on the top half.

notation $\mathbf{N} \leqslant \mathbf{M}$ to indicate that $\mathbf{N}$ is a subgraph of $\mathbf{M}$. Primed subgraphs will have the property that all of their lines contain sites with $i_1 \neq 0$. $N_-$ will be the total flux into sites of $\partial\Lambda$ with negative spins.

The combinatoric factors are such that

$$\sum_{\substack{\mathbf{n}' \leqslant \mathbf{m} \\ \partial\mathbf{n}' \backslash (\partial\Lambda U P_0) = \phi}} \prod_{b \in B'} \binom{m_b}{n'_b} (-1)^{n'_-}$$

equals

$$|\{\mathbf{N}' \leqslant \mathbf{M} \mid \partial\mathbf{N}' \backslash (\partial\Lambda U P_0) = \phi, N'_- \text{ is even}\}|$$
$$-|\{\mathbf{N}' \leqslant \mathbf{M} \mid \partial\mathbf{N}' \backslash (\partial\Lambda U P_0) = \phi, N'_- \text{ is odd}\}|$$

(Here $|A|$ denotes the cardinality of the set $A$.)

Our assumption on $\mathbf{m}$ implies that there exists $\mathbf{K}' \leqslant \mathbf{M}$ with $\partial\mathbf{K}'$ consisting of two sites: one an element of $\partial\Lambda \backslash P_0$, and the other an element of $P_0$.

We may use $\mathbf{K}'$ to set up a bijection between the above two collections. Define

$$\Delta_{\mathbf{K}'} : \{\mathbf{N}' \leqslant \mathbf{M} \mid \partial\mathbf{N}' \backslash (\partial\Lambda U P_0) = \phi, N'_- \text{ is even}\}$$
$$\to \{\mathbf{N}' \leqslant \mathbf{M} \mid \partial\mathbf{N}' \backslash (\partial\Lambda U P_0) = \phi, N'_- \text{ is odd}\}$$

via $\Delta_{\mathbf{K}'}(\mathbf{N}') = \mathbf{N}'\Delta\mathbf{K}'$.

The map $\Delta_{\mathbf{K}'}$ changes the value of $N'_-$ by exactly one and is clearly a bijection, thus proving the claim.

We are left with graphs $\mathbf{m}$ that contains no path between $P_0$ and $\partial\Lambda \backslash P_0$. Moreover, all of these graphs contribute to the sum with a positive sign. To see this, note that from flux conservation, any sources must occur in pairs, and that the above condition precludes a negative boundary spin from being connected to a positive one.

The restriction on $\mathbf{m}$ may be given a geometric interpretation as follows: On each bond $b$ with $m_b = 0$, place a plaquette on the midpoint of the bond, oriented such that $b$ is perpendicular to the surface of the plaquette. (In $d$ dimensions, the plaquettes are $(d-1)$-dimensional hypersquares.) Since there is no connection between $P_0$ and $\partial\Lambda \backslash P_0$, these plaquettes must link up to form a surface, which we will call a "null surface," separating these sets. Note that, in particular, the boundary spins in the $i_1 = 1$ layer are separated from $P_0$. Thus, the null surface is "tied down" at the box's edge at $i_1 = 1/2$. We restrict our attention to null surfaces which "enclose no volume." These are null surfaces with the property that every site $i \in \Lambda_{L,M}$ may be connected to either $\partial\Lambda \backslash P_0$ or to $P_0$ by a path which does not cross the null surface. A two-dimensional null surface is shown in Fig. 2.

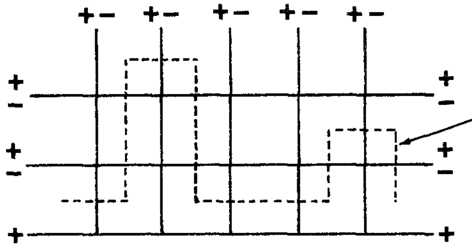


Fig. 2. A two-dimensional null surface.

Hence the partition function $Z^{\pm}_{L,M}$ may be written

$$Z^{\pm}_{L,M} = \sum_{\partial\mathbf{m}\setminus\partial\Lambda=\phi}^{*} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\setminus(\partial\Lambda\, U P_0)=\phi}} \prod_{b\in B'} \binom{m_b}{n'_b} \tag{2.3}$$

where the asterisk (*) refers to the restriction that **m** contains a null surface separating $\partial\Lambda\setminus P_0$ from $P_0$.

In general, a given configuration **m** may contain several such null surfaces. However, it will contain only one uppermost null surface, characterized by the following property:

Let $S$ be a null surface separating $P_0$ from $\partial\Lambda\setminus P_0$, and suppose that $S$ consists of plaquettes $p_1, \ldots, p_s$ breaking bonds $b_1, \ldots, b_s$. We will say that $S$ is the uppermost null surface appearing in **m** if for all $i = 1, \ldots, s$, $b_i$ contains exactly one site that is connected to $\partial\Lambda\setminus P_0$ by a path in **m**.

This definition of the uppermost null surface appearing in **m** may be visualized as follows. Let $C_{\mathbf{m}}(\partial\Lambda\setminus P_0)$ be the set of sites that may be reached from $\partial\Lambda\setminus P_0$ by paths in **m**. Of course, $\partial\Lambda\setminus P_0 \subseteq C_{\mathbf{m}}(\partial\Lambda\setminus P_0)$. Let $C^V_{\mathbf{m}}(\partial\Lambda\setminus P_0)$ be the volume obtained by taking the union of unit cells centered around elements of $C_{\mathbf{m}}(\partial\Lambda\setminus P_0)$. The boundary of this volume will consist of a null surface separating $\partial\Lambda\setminus P_0$ from $P_0$, plus a number of isolated "bubbles" of null surface, which may be large depending on the configuration **m**. Geometrically, the uppermost null surface is the boundary of $C^V_{\mathbf{m}}(\partial\Lambda\setminus P_0)$—excluding all of the bubbles.

The main result presented here is that the uppermost null surfaces fluctuate to infinity precisely at the roughening transition. It has already been shown that one may use this construction to give a graphical proof of van Beijeren's theorem on the existence of states that are not translation invariant.[14] We submit that the random currents, which are bounded by null surfaces, describe in a rather exact sense the elementary excitations which produce spin correlations.

## 3. CORRESPONDENCE WITH THE ROUGHENING TRANSITION

In this section we will show the connection between the uppermost null surfaces found in the last section and the roughening transition.

Clearly, the uppermost null surface (u.n.s.) in $\Lambda_{L,M}$ intersects the box $\Lambda_{N,N}$ if and only if there exists a site $i \in \Lambda_{N,N}$ and a path $\Gamma_i$ from $i$ to $\partial\Lambda_{L,M}\backslash P_0$ such that $\Gamma_i$ does not cross the surface.

Let $R_{L,M}(N)$ be the probability that the u.n.s. in $\Lambda_{L,M}$ intersects $\Lambda_{N,N}$. By definition

$$R_{L,M}(N) = \frac{\sum^{**}_{\partial\mathbf{m}\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\backslash(\partial\Lambda\, UP_0)=\phi}} \prod_{b\in B'} \binom{m_b}{n'_b}}{\sum^{*}_{\partial\mathbf{m}\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\backslash(\partial\Lambda\, UP_0)=\phi}} \prod_{b\in B'} \binom{m_b}{n'_b}} \tag{3.1}$$

The single-asterisk summation satisfies the same restriction as in (2.3), and the double-asterisk summation satisfies the additional restriction that the u.n.s. intersects $\Lambda_{N,N}$.

We prove as our main result:

**Proposition 3.1.** For any temperature such that the pressure $P = (1/\beta)\lim_{\Lambda\to\infty}(1/|\Lambda|)\ln Z$ of a nearest-neighbor Ising model is differentiable, we have

(i) $$\varliminf_{L\to\infty}\ \varliminf_{M\to\infty} R_{L,M}(N) = 0$$

for all $N$ implies that the $\langle\cdot\rangle^{\pm}$ state is translation invariant, and conversely

(ii) $$\varlimsup_{L\to\infty}\ \varlimsup_{M\to\infty} R_{L,M}(N) > 0$$

for some $N$, implies that the state $\langle\cdot\rangle^{\pm}$ is not translation invariant.

In the proof, we will make use of the following result due to Lebowitz.[15]

**Theorem** (Lebowitz). Let $J_{ij}$ be a finite-range, translation invariant interaction such that $J_{ij} > 0$ for $|i-j| = 1$, and let $h = 0$. Then the existence of $(dP/d\beta)|_{\beta_0}$ implies that all translation invariant states agree with the plus state on even correlation functions at inverse temperature $\beta_0$.

Before proving Proposition 3.1, the main ideas behind the construction will be summarized. Graphical methods have permitted us to express the partition function in the manifestly positive form (2.3). Each $\mathbf{m}$ contributing to the sum contains a unique uppermost null surface $S$. The partition function may be evaluated by summing first over configurations $\mathbf{m}$ satisfying "$S$ is the uppermost null surface appearing in $\mathbf{m}$," and then over $S$. Consider "unfolding" the system by undoing the reflection $(i_1, i_2, \ldots, i_d)$

$\rightarrow (-i_1, i_2, \ldots, i_d)$ for $i_1 < 0$. The null surface $S$ together with its reflection $S^R$ combine to separate a "fat" $(d-1)$-dimensional system surrounding the origin from the rest of the $d$-dimensional system. This procedure is illustrated in Fig. 3. The choice of the uppermost null surface insures that the partition function for the central region is unconstrained.

We now take the infinite volume limit, and consider two cases. First suppose that the uppermost null surface fluctuates to infinity. In this case, the central system becomes $d$ dimensional, and is between the plus and "free" states in the FKG sense. Correlation inequalities and the Lebowitz theorem may be combined to show that the resulting state is translation invariant.

Now suppose that the uppermost null surface has a nonzero probability of passing a finite distance from the plane $P_0$. In this case, stable local interfaces exist and it is easy to show that the state cannot be translation invariant.

The first step in proving Proposition 3.1 is to derive an expression for $\langle \sigma_y \sigma_{y'} \rangle^{\pm}_{L,M}$, where $y = (y_1, y_2, \ldots, y_d)$ is any site with $y_1 > 0$, and $y' = (-y_1, y_2, \ldots, y_d)$.

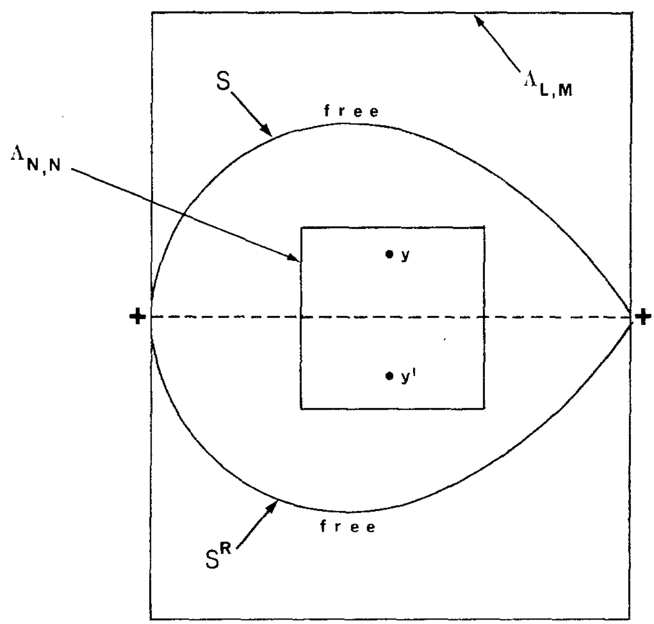


Fig. 3. The "+, free" boundary conditions.

In analogy with (2.2), we have

$$Z^{\pm}_{L,M}\langle\sigma_y\sigma_{y'}\rangle^{\pm}_{L,M} = \sum_{\partial\mathbf{m}\setminus\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\setminus(\partial\Lambda\, UP_0)=y'}} \prod_{b\in B'} \binom{m_b}{n'_b}(-1)^{n'_-} \tag{3.2}$$

As before, if $\mathbf{m}$ does not contain a null surface separating $\partial\Lambda\setminus P_0$ from $P_0$, the net contribution is zero. For graphs $\mathbf{m}$ containing a null surface, the contribution to (3.2) is positive if the u.n.s. passes above $y$, but negative if it passes below $y$, since in the latter case $y'$ must be connected to a source on the negative boundary.

Hence, (3.2) may be written

$$\sum_{\partial\mathbf{m}\setminus\partial\Lambda=\phi}' W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\setminus(\partial\Lambda\, UP_0)=y'}} \prod_{b\in B'} \binom{m_b}{n'_b}$$
$$- \sum_{\partial\mathbf{m}\setminus\partial\Lambda=\phi}'' W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\setminus(\partial\Lambda\, UP_0)=y'}} \prod_{b\in B'} \binom{m_b}{n'_b} \tag{3.3}$$

In the single primed summation, the u.n.s. passes above $y$, while in the double primed summation it passes below $y$.

We may now use the symmetric difference trick to write the second term as

$$\sum_{\partial\mathbf{m}\setminus\partial\Lambda=\phi}''' W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\setminus(\partial\Lambda\, UP_0)=\phi}} \prod_{b\in B'} \binom{m_b}{n'_b} \tag{3.4}$$

The triple primed summation includes only graphs $\mathbf{m}$ such that the u.n.s. passes below $y$ and $\mathbf{m}$ contains at least one path from $y$ to $\partial\Lambda\setminus P_0$.

Finally,

$$\langle\sigma_y\sigma_{y'}\rangle^{\pm}_{L,M} = \frac{\displaystyle\sum_{\partial\mathbf{m}\setminus\partial\Lambda=\phi}' W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\setminus(\partial\Lambda\, UP_0)=y'}} \prod_{b\in B'} \binom{m_b}{n'_b}}{\displaystyle\sum_{\partial\mathbf{m}\setminus\partial\Lambda=\phi}^{*} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\setminus(\partial\Lambda\, UP_0)=\phi}} \prod_{b\in B'} \binom{m_b}{n'_b}}$$
$$- \operatorname{Prob}(y\to\partial\Lambda\setminus P_0 \mid \exists \text{ a n.s.}) \tag{3.5}$$

The last term is by definition the ratio of (3.4) to (2.3). Since the source constraints in numerator and denominator are the same, we have expressed it as the probability that $\mathbf{m}$ connects $y$ to $\partial\Lambda\setminus P_0$, conditioned on the existence of a null surface separating $P_0$ from $\partial\Lambda\setminus P_0$.

The proof of Proposition 3.1 relies on the following two lemmas, which are based on (3.5).

**Lemma 3.2.** For any $N < \min(L, M)$ such that $y \in \Lambda_{N,N}$ we have

$$\langle \sigma_y \sigma_{y'} \rangle^{\pm}_{L,M} \geqslant \langle \sigma_y \sigma_{y'} \rangle^{\text{free}}_{N,N} (1 - R_{L,M}(N)) - R_{L,M}(N)$$

**Lemma 3.3.** Let $N$ be as in Lemma 3.2. Then

$$\langle \sigma_y \sigma'_y \rangle^{\pm}_{L,M} \leqslant \langle \sigma_y \sigma'_y \rangle^{+}_{L,M} - \text{Prob}(y \to \partial\Lambda \backslash P_0 \,|\, \exists \text{ a n.s.})$$

The proofs of these lemmas are deferred to the end of this section. We first show how Proposition 3.1 follows from these results. An outline of the argument will be given, followed by the proof.

If the probability of the uppermost null surface intersecting a finite box is vanishingly small, then Lemmas 3.2 and 3.3 combined with the Lebowitz theorem show that $\langle \sigma_y \sigma_{y'} \rangle^{\pm} = \langle \sigma_y \sigma_{y'} \rangle^{+}$. Correlation inequalities may now be used to deduce that the magnetization vanishes, and thus that the state is translation invariant.

If, on the other hand, there is a positive probability of the uppermost null surface passing through a finite box, Lemma 3.3 shows that $\langle \sigma_y \sigma_{y'} \rangle^{\pm} \neq \langle \sigma_y \sigma_{y'} \rangle^{+}$. The Lebowitz theorem may now be used to conclude that the $\langle \cdot \rangle^{\pm}$ state is not translation invariant. The details of the proof will now be given.

*Proof of Proposition 3.1* (assuming the lemmas).

(i) Suppose that $\beta$ is such that $dP/d\beta$ exists and that

$$\varliminf_{L\to\infty} \varliminf_{M\to\infty} R_{L,M}(N) = 0 \qquad \text{for all } N$$

Let $\epsilon > 0$, and let $y$ be any site with $y_1 > 0$. Choose $N$ so large that $y \in \Lambda_{N,N}$ and $\langle \sigma_y \sigma_{y'} \rangle^{\text{free}} - \langle \sigma_y \sigma_{y'} \rangle^{\text{free}}_{N,N} < \epsilon/3$.

By hypothesis, there exist subsequences $\{M_n\}$ and $\{L_k\}$ such that $\lim_{k\to\infty} \lim_{n\to\infty} R_{L_k,M_n}(N) = 0$. Fix a subsequence, and choose $K$ such that $k > K$ implies $\lim_{n\to\infty} R_{L_k,M_n}(N) < \epsilon/3$.

Let $k > K$. From Lemma (3.2),

$$\langle \sigma_y \sigma_{y'} \rangle^{\pm}_{L_k,M_n} \geqslant (\langle \sigma_y \sigma_{y'} \rangle^{\text{free}} - \epsilon/3)(1 - R_{L_k,M_n}(N)) - R_{L_k,M_n}(N), \quad \text{and hence,}$$

$$\lim_{n\to\infty} \langle \sigma_y \sigma_{y'} \rangle^{\pm}_{L_k,M_n} \geqslant \langle \sigma_y \sigma_{y'} \rangle^{\text{free}} - \epsilon$$

Since $\lim_{L\to\infty} \lim_{M\to\infty} \langle \sigma_y \sigma_{y'} \rangle^{\pm}_{L,M}$ is known to exist from correlation inequalities,[2,6] we can conclude

$$\langle \sigma_y \sigma_{y'} \rangle^{\pm} \geqslant \langle \sigma_y \sigma_{y'} \rangle^{\text{free}}$$

On the other hand, Lemma 3.3 immediately shows that

$$\langle \sigma_y \sigma_{y'} \rangle^{\pm} \leqslant \langle \sigma_y \sigma_{y'} \rangle^{+}$$

Since the plus and free states are both translation invariant, we have from Lebowitz's theorem that

$$\langle \sigma_y \sigma_{y'} \rangle^{\pm} = \langle \sigma_y \sigma_{y'} \rangle^{+}$$

The new Lebowitz inequality[15] implies that

$$\begin{aligned} \langle \sigma_y \sigma_{y'} \rangle^{+} - \langle \sigma_y \sigma_{y'} \rangle^{\pm} &\geqslant |\langle \sigma_{y'} \rangle^{+} \langle \sigma_y \rangle^{\pm} - \langle \sigma_{y'} \rangle^{\pm} \langle \sigma_y \rangle^{+}| \\ &= \langle \sigma_y \rangle^{+} |\langle \sigma_y \rangle^{\pm} - \langle \sigma_y' \rangle^{\pm} | \end{aligned}$$

Hence $\langle \sigma_y \rangle^{\pm} = \langle \sigma_{y'} \rangle^{\pm}$.

Now, since $\langle \sigma_y \rangle^{\pm} \geqslant 0$ and $\langle \sigma_{y'} \rangle^{\pm} \leqslant 0$, we have $\langle \sigma_y \rangle^{\pm} = 0 = \langle \sigma_{y'} \rangle^{\pm}$.

This shows that $\langle \sigma_y \rangle^{\pm} = 0$ for all $y$ with $y_1 \neq 0$, but it is easy to see that this condition implies $\langle \sigma_y \rangle^{\pm} = 0$ for all $y$.

Hence the $\langle \cdot \rangle^{\pm}$ state is translation invariant.

(ii) Now suppose that $dP/d\beta$ exists and that $\overline{\lim}_{L\to\infty} \overline{\lim}_{M\to\infty} R_{L,M}(N) = \delta > 0$ for some $N$.

Then there exists $y \in \Lambda_{N,N}$ such that

$$\overline{\lim_{L\to\infty}}\ \overline{\lim_{M\to\infty}} \frac{\sum^{y}_{\partial \mathbf{m} \setminus \partial \Lambda = \phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}' \leqslant \mathbf{m} \\ \partial \mathbf{n}' \setminus (\partial \Lambda\, U P_0) = \phi}} \prod_{b \in B'} \binom{m_b}{n_b'}}{\sum^{*}_{\partial \mathbf{m} \setminus \partial \Lambda = \phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}' \leqslant \mathbf{m} \\ \partial \mathbf{n}' \setminus (\partial \Lambda\, U P_0) = \phi}} \prod_{b \in B'} \binom{m_b}{n_b'}} \geqslant \eta > 0$$

for some $\eta$. In the numerator, the u.n.s. is constrained to pass immediately below $y$. From the definition of u.n.s. this condition forces $\mathbf{m}$ to connect $y$ to $\partial\Lambda \setminus P_0$. Hence $\overline{\lim}_{L\to\infty}\overline{\lim}_{M\to\infty}\mathrm{Prob}(y \to \partial\Lambda \mid \exists \text{ a n.s.}) \geqslant \eta$, and Lemma 3.3 shows that

$$\langle \sigma_y \sigma_{y'} \rangle^{\pm} \leqslant \langle \sigma_y \sigma_{y'} \rangle^{+} - \eta$$

Hence $\langle \cdot \rangle^{\pm}$ is not translation invariant. ■

*Proof of Lemma 3.2.* Our starting point is Eq. (3.5). If $y \to \partial\Lambda \setminus P_0$, and $y \in \Lambda_{N,N}$, then the u.n.s. must, by definition, intersect $\Lambda_{N,N}$. Hence

$$\mathrm{Prob}(y \to \partial\Lambda \setminus P_0 \mid \exists \text{ a n.s.}) \leqslant R_{L,M}(N)$$

It is, therefore, enough to show

$$\frac{\displaystyle\sum'_{\partial\mathbf{m}\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\backslash(\partial\Lambda\, UP_0)=y'}} \prod_{b\in B'} \binom{m_b}{n'_b}}{\displaystyle\sum^*_{\partial\mathbf{m}\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\backslash(\partial\Lambda\, UP_0)=\phi}} \prod_{b\in B'} \binom{m_b}{n'_b}} \geqslant \langle\sigma_y\sigma_{y'}\rangle^{\text{free}}_{N,N}(1-R_{L,M}(N)) \tag{3.6}$$

The asterisk summation obeys the restriction that there exists a null surface separating $P_0$ from $\partial\Lambda\backslash P_0$, and in the primed summation, the surface is constrained to pass above $y$.

The numerator in the left-hand side of (3.6) is not smaller than

$$\sum^{N^{\sim}}_{\partial\mathbf{m}\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\backslash(\partial\Lambda\, UP_0)=y'}} \prod_{b\in B'} \binom{m_b}{n'_b}$$

where the symbol $N^{\sim}$ denotes the restriction that the u.n.s. does not intersect $\Lambda_{N,N}$. Hence the left-hand side of (3.6) is bounded below by

$$\frac{\displaystyle\sum^{N^{\sim}}_{\partial\mathbf{m}\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}'\backslash(\partial\Lambda\, UP_0)=y'}} \prod_{b\in B'} \binom{m_b}{n'_b}}{\displaystyle\sum^{N^{\sim}}_{\partial\mathbf{m}\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'\leqslant\mathbf{m}\\ \partial\mathbf{n}\backslash(\partial\Lambda\, UP_0)=\phi}} \prod_{b\in B'} \binom{m_b}{n'_b}} (1-R_{L,M}(N)) \tag{3.7}$$

These sums will now be evaluated by conditioning on the event "the u.n.s. appearing in the configuration $\mathbf{m}$ is $S$," and then summing over surfaces $S$ which do not intersect $\Lambda_{N,N}$. Further, we will use $S$ to divide $\Lambda_{L,M}$ into two regions, the region above $S$ (denoted by the subscript $a$) and the region below $S$ (denoted by $d$). The restriction "$S$ is the u.n.s." introduces a constraint on the allowable configurations of fluxes above $S$, but the region below $S$ is unconstrained.

Equation (3.7) becomes

$$\frac{\displaystyle\sum_S \sum^{S=\text{u.n.s.}}_{\partial\mathbf{m}_a\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'_a\leqslant\mathbf{m}_a\\ \partial\mathbf{n}'_a\backslash\partial\Lambda=\phi}} \prod_{b\in B'} \binom{m_{b_a}}{n'_{b_a}} \sum_{\partial\mathbf{m}_d\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'_d\leqslant\mathbf{m}_d\\ \partial\mathbf{n}'_d\backslash P_0=y'}} \prod_{b\in B'} \binom{m_{b_d}}{n'_{b_d}}}{\displaystyle\sum_S \sum^{S=\text{u.n.s.}}_{\partial\mathbf{m}_a\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'_a\leqslant\mathbf{m}_a\\ \partial\mathbf{n}'_a\backslash\partial\Lambda=\phi}} \prod_{b\in B'} \binom{m_{b_a}}{n'_{b_a}} \sum_{\partial\mathbf{m}_d\backslash\partial\Lambda=\phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}'_d\leqslant\mathbf{m}_d\\ \partial\mathbf{n}'_d\backslash P_0=\phi}} \prod_{b\in B'} \binom{m_{b_d}}{n'_{b_d}}}$$

$$\times(1-R_{L,M}(N)) \tag{3.8}$$

Now write

$$\sum_{\substack{\mathbf{n}'_d \leqslant \mathbf{m}_d \\ \partial \mathbf{n}'_d \setminus P_0 = y'}} \prod_{b \in B'} \binom{m_{b_d}}{n'_{b_d}} = \sum_{\substack{\mathbf{n}'_d \leqslant \mathbf{m}_d \\ \partial \mathbf{n}'_d \setminus P_0 = \phi}} \prod_{b \in B'} \binom{m_{b_d}}{n'_{b_d}} \left[ \frac{\displaystyle\sum_{\substack{\mathbf{n}'_d \leqslant \mathbf{m}_d \\ \partial \mathbf{n}'_d \setminus P_0 = y'}} \prod_{b \in B'} \binom{m_{b_d}}{n'_{b_d}}}{\displaystyle\sum_{\substack{\mathbf{n}'_d \leqslant \mathbf{m}_d \\ \partial \mathbf{n}'_d \setminus P_0 = \phi}} \prod_{b \in B'} \binom{m_{b_d}}{n'_{b_d}}} \right] \tag{3.9}$$

If we now "unfold the system, i.e., undo the reflection $(i_1, i_2, \ldots, i_d) \to (-i_1, i_2, \ldots, i_d)$ for $i_1 < 0$, the expression in brackets becomes $\langle \sigma_y \sigma_{y'} \rangle^{+,\text{free}}_{\text{below } S}$. Let $S^R$ denote the reflection of $S$ in the plane $P_0$. Then "below $S$" indicates the symmetric region bounded by $S$, $S^R$, and $\partial\Lambda$. The boundary conditions "$+$, free" are illustrated in Fig. 3. They consist of plus boundary conditions on the plane $P_0$ and free boundary conditions at the surfaces $S$ and $S^R$.

From the GKS inequalities[16] we have

$$\langle \sigma_y \sigma_{y'} \rangle^{+,\text{free}}_{\text{below } S} \geqslant \langle \sigma_y \sigma_{y'} \rangle^{\text{free}}_{N,N} \tag{3.10}$$

Substituting (3.10) in (3.9), and the result in (3.8) establishes the lemma. ∎

*Proof of Lemma 3.3.* From (3.5), it is enough to show that

$$\frac{\displaystyle\sum'_{\partial \mathbf{m} \setminus \partial\Lambda = \phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}' \leqslant \mathbf{m} \\ \partial \mathbf{n}' \setminus (\partial\Lambda\, U P_0) = y'}} \prod_{b \in B'} \binom{m_b}{n'_b}}{\displaystyle\sum^*_{\partial \mathbf{m} \setminus \partial\Lambda = \phi} W(\mathbf{m}) \sum_{\substack{\mathbf{n}' \leqslant \mathbf{m} \\ \partial \mathbf{n}' \setminus (\partial\Lambda\, U P_0) = \phi}} \prod_{b \in B'} \binom{m_b}{n'_b}} \leqslant \langle \sigma_y \sigma_{y'} \rangle^{+}_{L,M} \tag{3.11}$$

The left-hand of (3.11) is bounded above by the expression one obtains by replacing the starred summation in the denominator by a primed summation with the same source constraints. The resulting expression may now be evaluated by the method used to obtain (3.8). An application of the upper bound

$$\langle \sigma_y \sigma_{y'} \rangle^{+,\text{free}}_{\text{below } S} \leqslant \langle \sigma_y \sigma_{y'} \rangle^{+}_{L,M}$$

leads immediately to (3.11). ∎

## ACKNOWLEDGMENT

It is a pleasure to thank Michael Aizenman and Jean Bricmont for valuable conversations.

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